

DEPARTMENT OF MATHEMATICS & STATISTICS
COLLEGE OF SCIENCES
OLD DOMINION UNIVERSITY
NORFOLK, VIRGINIA 23529

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**THEORETICAL STUDIES OF A MOLECULAR BEAM
GENERATOR**

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By

John Heinbockel, Principal Investigator

Progress Report

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Dr. Sang H. Choi, Technical Monitor
SSD-High Energy Science Branch

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THEORETICAL STUDIES OF A MOLECULAR BEAM GENERATOR

Introduction

At present no adequate computer code exists for predicting the effects of thermal nonequilibrium on the flow quality of a converging-diverging N_2 nozzle. It is the purpose of this research to develop such a code and then perform parametric studies to determine the effects of intermolecular forces (high gas pressure) and thermal nonequilibrium (the splitting of temperature into a vibrational and rotational-translational excitation) upon the flow quality.

The two models to be compared are given below. See Appendix A for nomenclature and additional relationships.

Model 1 (Equilibrium Model)

Continuity Equation

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \vec{V} = 0 \quad (1)$$

Momentum Equations

$$\rho \frac{D\vec{V}}{Dt} = \rho \vec{b} + \nabla \cdot (\sigma_{ij}) \quad (2)$$

Energy Equation

$$\frac{\partial e_t}{\partial t} + \nabla \cdot (e_t \vec{V}) = \frac{\partial Q}{\partial t} - \nabla \vec{q} + \rho \vec{b} \cdot \vec{V} + \nabla \cdot (\sigma_{ij} \cdot \vec{V}) \quad (3)$$

Equation of State

$$P = (\gamma - 1)\rho e_t, \quad \gamma = \frac{C_p}{C_v}, \quad C_p = \frac{\gamma R}{\gamma - 1} \quad (4)$$

Model 2 (Nonequilibrium Model)

Continuity Equation

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \vec{V} = 0 \quad (5)$$

Momentum Equations

$$\rho \frac{D\vec{V}}{Dt} = \rho \vec{V} + \nabla \cdot (\sigma_{ij}) \quad (6)$$

Energy Equations

$$\begin{aligned} \frac{\partial e_r}{\partial t} + \nabla \cdot (e_r \vec{V}) &= \frac{\partial Q}{\partial t} - \nabla \cdot \vec{q}_{rt} + \nabla \cdot (\sigma_{ij} \cdot \vec{V}) - \rho C_{vv} X \\ \frac{\partial e_v}{\partial t} + \nabla \cdot (e_v \vec{V}) &= - \nabla \cdot \vec{q}_v + \rho C_{vv} X \end{aligned} \quad (7)$$

The above equations express the compressible Navier Stokes equations which govern the basic dynamics of compressible fluid motion. In these equations we will assume that there are no body forces $\vec{b} = 0$, and there are no external heat sources $Q = 0$. In the above models the following relations hold

$$e_t = e_r + e_v, \quad e_r = \rho C_{vrt} T + \rho V^2/2, \quad e_v = \rho C_{vv} T_v \quad (8)$$

$$C_v = C_{vrt} + C_{vv}|_{T=T_*}, \quad C_{vrt} = \frac{5}{2} R, \quad \phi = \frac{h\nu}{k} \quad (9)$$

$$C_{vv} = \frac{k}{m} \left(\frac{\phi}{T_v} \right)^2 \exp \left(\frac{\phi}{T_v} \right) \left(\exp \left(\frac{\phi}{T_v} \right) - 1 \right)^{-2} \quad (10)$$

$$\vec{q}_{rt} = -K_{rt} \nabla T \quad \vec{q}_v = -K_v \nabla T_v \quad (11)$$

$$K = K_v + K_{rt}, \quad K_v = \eta C_{vv}, \quad K_{rt} = \frac{19\eta k}{4m}, \quad \eta = \frac{c_1 g_c T^{3/2}}{T + c_2} \quad (12)$$

$$X = \frac{T_v^2}{\phi \tau} \left[\frac{1 - e^{-\phi/T_*}}{1 - e^{-\phi/T}} \right] \left\{ \exp \left[\phi \left(\frac{1}{T_v} - \frac{1}{T} \right) - 1 \right] \right\} \quad (13)$$

$$P(atm)\tau = \frac{1.402(10^{11}) \left(\frac{T}{3.12(10^7)} \right)^{2/3} \exp \left[\left(\frac{3.12(10^7)}{T} \right)^{1/3} - \frac{95.9}{T} \right]}{(1 + \text{erf}(\xi)) \sinh \left(\frac{1698}{T} \right)} \quad (14)$$

$$\xi = \left(\frac{4.88(10^5)}{T} \right)^{1/6} \left(1 - \left(\frac{70.6}{T} \right)^{2/3} \right) \quad (15)$$

where η is the viscosity given by Sutherland formula with

$$c_1 = 2.16(10^{-8}) * 1.488, \quad c_2 = 184.0, \quad \text{and} \quad g_c = \frac{5}{2}R \text{ for } N_2.$$

Conservative Equations

The continuity equation and energy equation are examples of scalar conservation laws which have the general form

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot \vec{b} = 0 \quad (16)$$

where α is a scalar and \vec{b} is a vector. In Cartesian coordinates we have for the continuity equation

$$\alpha = \rho \quad \text{and} \quad \vec{b} = \rho V_x \hat{e}_1 + \rho V_y \hat{e}_2 + \rho V_z \hat{e}_3 \quad (17)$$

and for the energy equation we have $\alpha = e_t$ and

$$\begin{aligned} \vec{b} = & \left[(e_t + P)V_1 - \sum_{i=1}^3 V_i \tau_{xi} + q_x \right] \hat{e}_1 + \\ & \left[(e_t + P)V_2 - \sum_{i=1}^3 V_i \tau_{yi} + q_y \right] \hat{e}_2 + \\ & \left[(e_t + P)V_3 - \sum_{i=1}^3 V_i \tau_{zi} + q_z \right] \hat{e}_3 \end{aligned} \quad (18)$$

where

$$e_t = \rho e + \rho(V_1^2 + V_2^2 + V_3^2)/2.$$

In general orthogonal coordinates (x_1, x_2, x_3) the equation (16) is written in the form

$$\frac{\partial}{\partial t}((h_1 h_2 h_3 \alpha)) + \frac{\partial}{\partial x_1}((h_2 h_3 b_1)) + \frac{\partial}{\partial x_2}((h_1 h_3 b_2)) + \frac{\partial}{\partial x_3}((h_1 h_2 b_3)) = 0. \quad (19)$$

where h_1, h_2, h_3 are the scale factors obtained from the transformation equations to the general orthogonal coordinates.

The momentum equations are examples of a vector conservation law having the general form

$$\frac{\partial \vec{a}}{\partial t} + \nabla \cdot (\mathbf{T}) = 0 \quad (20)$$

where \vec{a} is a vector and \mathbf{T} is a symmetric tensor

$$\mathbf{T} = \sum_{k=1}^3 \sum_{j=1}^3 T_{jk} \hat{e}_j \hat{e}_k. \quad (21)$$

In general coordinates we have for the momentum equations

$$\vec{a} = \rho \vec{V} \quad \text{and} \quad T_{ij} = \rho V_i V_j + P \delta_{ij} - \tau_{ij}.$$

In general orthogonal coordinates (x_1, x_2, x_3) the conservation law (19) can be written

$$\frac{\partial}{\partial t}((h_1 h_2 h_3 \vec{a})) + \frac{\partial}{\partial x_1}((h_2 h_3 \mathbf{T} \cdot \hat{\mathbf{e}}_1)) + \frac{\partial}{\partial x_2}((h_1 h_3 \mathbf{T} \cdot \hat{\mathbf{e}}_2)) + \frac{\partial}{\partial x_3}((h_1 h_2 \mathbf{T} \cdot \hat{\mathbf{e}}_3)) = 0 \quad (22)$$

Example 1 Cartesian Coordinates

In Cartesian coordinates the model 1 can be written in the strong conservative form

$$\frac{\partial U}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} = 0 \quad (23)$$

where

$$U = \begin{bmatrix} \rho \\ \rho V_x \\ \rho V_y \\ \rho V_z \\ e_t \end{bmatrix} \quad (24)$$

$$E = \begin{bmatrix} \rho V_x \\ \rho V_x^2 + P - \tau_{xx} \\ \rho V_x V_y - \tau_{xy} \\ \rho V_x V_z - \tau_{xz} \\ (e_t + P)V_x - V_x \tau_{xx} - V_y \tau_{xy} - V_z \tau_{xz} + q_x \end{bmatrix} \quad (25)$$

$$F = \begin{bmatrix} \rho V_y \\ \rho V_x V_y - \tau_{xy} \\ \rho V_y^2 + P - \tau_{yy} \\ \rho V_x V_z - \tau_{yz} \\ (e_t + P)V_y - V_x \tau_{yx} - V_y \tau_{yy} - V_z \tau_{yz} + q_y \end{bmatrix} \quad (26)$$

$$G = \begin{bmatrix} \rho V_z \\ \rho V_x V_z - \tau_{xz} \\ \rho V_y V_z - \tau_{yz} \\ \rho V_z^2 + P - \tau_{zz} \\ (e_t + P)V_z - V_x \tau_{zx} - V_y \tau_{zy} - V_z \tau_{zz} + q_z \end{bmatrix} \quad (27)$$

where the shear stresses are given by

$$\tau_{ij} = \eta(V_{i,j} + V_{j,i}) + \delta_{ij} \lambda V_{k,k}$$

for $i, j, k = 1, 2, 3$.

Example 2 Cylindrical Coordinates

The transformation equations to cylindrical coordinates are given by

$$x = r \cos \theta$$

$$y = r \sin \theta$$

$$z = z$$

and have unit basis vectors

$$\hat{\mathbf{e}}_1 = \hat{\mathbf{e}}_r = \cos \theta \hat{\mathbf{e}}_1 + \sin \theta \hat{\mathbf{e}}_2$$

$$\hat{\mathbf{e}}_2 = \hat{\mathbf{e}}_\theta = -\sin \theta \hat{\mathbf{e}}_1 + \cos \theta \hat{\mathbf{e}}_2$$

$$\hat{\mathbf{e}}_3 = \hat{\mathbf{e}}_z = \hat{\mathbf{e}}_3$$

and scale factors $h_1 = 1, h_2 = r, h_3 = 1$. Consequently, the continuity equation can be expressed

$$\frac{\partial(\rho r)}{\partial t} + \frac{\partial(r\rho V_r)}{\partial r} + \frac{\partial(\rho V_\theta)}{\partial \theta} + \frac{\partial(r\rho V_z)}{\partial z} = 0 \quad (28)$$

and the energy equation has the form

$$\begin{aligned} \frac{\partial(re_t)}{\partial t} &= \frac{\partial}{\partial r}((r[(e_t + P)V_r - V_r\tau_{rr} - V_\theta\tau_{r\theta} - V_z\tau_{rz} + q_r])) + \\ &\quad \frac{\partial}{\partial \theta}((r[(e_t + P)V_\theta - V_r\tau_{\theta r} - V_\theta\tau_{\theta\theta} - V_z\tau_{\theta z} + q_\theta])) + \\ &\quad \frac{\partial}{\partial z}((r[(e_t + P)V_z - V_r\tau_{zr} - V_\theta\tau_{z\theta} - V_z\tau_{zz} + q_z])) = 0 \end{aligned} \quad (29)$$

The momentum equations have the form

$$\begin{aligned} \frac{\partial}{\partial t}((r\rho V_r)) + \frac{\partial}{\partial r}((rT_{rr})) + \frac{\partial}{\partial \theta}((T_{r\theta})) - T_{\theta\theta} + \frac{\partial}{\partial z}((rT_{rz})) &= 0 \\ \frac{\partial}{\partial t}((r\rho V_\theta)) + \frac{\partial}{\partial r}((rT_{\theta r})) + T_{r\theta} + \frac{\partial}{\partial \theta}(T_{\theta\theta}) + \frac{\partial}{\partial z}((rT_{\theta z})) &= 0 \\ \frac{\partial}{\partial t}((r\rho V_z)) + \frac{\partial}{\partial r}((rT_{rz})) + \frac{\partial}{\partial \theta}(T_{z\theta}) + \frac{\partial}{\partial z}((rT_{zz})) &= 0. \end{aligned} \quad (30)$$

For symmetry with respect to the θ variable we set all derivative terms with respect to theta equal to zero and consider only momentum in the r and z directions. Under these conditions the only stresses to consider are given by

$$\begin{aligned}\tau_{rr} &= 2\eta \frac{\partial V_r}{\partial r} + \lambda \left(\frac{1}{r} \frac{\partial(rV_r)}{\partial r} + \frac{\partial V_z}{\partial z} \right) \\ \tau_{\theta\theta} &= 2\eta \frac{V_r}{r} + \lambda \left(\frac{1}{r} \frac{\partial(rV_r)}{\partial r} + \frac{\partial V_z}{\partial z} \right) \\ \tau_{zz} &= 2\eta \frac{\partial V_z}{\partial z} + \lambda \left(\frac{1}{r} \frac{\partial(rV_r)}{\partial r} + \frac{\partial V_z}{\partial z} \right) \\ \tau_{rz} &= \tau_{zr} = \eta \left(\frac{\partial V_z}{\partial r} + \frac{\partial V_r}{\partial z} \right)\end{aligned}\tag{31}$$

and the above momentum equations reduce to

$$\begin{aligned}\frac{\partial}{\partial t}((r\rho V_r)) + \frac{\partial}{\partial r}((r[\rho V_r^2 + P - \tau_{rr}])) - P + \tau_{\theta\theta} + \frac{\partial}{\partial z}((r[\rho V_r V_z - \tau_{rz}])) &= 0 \\ \frac{\partial}{\partial t}((r\rho V_z)) + \frac{\partial}{\partial r}((r[\rho V_r V_z - \tau_{rz}])) + \frac{\partial}{\partial z}((r[\rho V_z^2 + P - \tau_{zz}])) &= 0.\end{aligned}\tag{32}$$

Method of Solution

In cylindrical coordinates, both the models 1 and 2 can be written in the weak conservative form

$$\frac{\partial U}{\partial t} + \frac{\partial E'}{\partial r} + \frac{\partial F'}{\partial z} + H = 0.\tag{33}$$

The nozzle boundary is described by some defining equation $r^* = f(z)$, $0 \leq z \leq b$ and therefore we can introduce the transformation equations

$$\begin{aligned}x &= \frac{z}{b} \\ y &= \frac{r}{r^*} = \frac{r}{f(xb)}\end{aligned}\tag{34}$$

The computational domain then becomes the x, y domain where $0 \leq x \leq 1$ and $0 \leq y \leq 1$ and the weak conservative form given by equation (33) can be written in the form

$$\frac{\partial U}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + H = 0\tag{35}$$

where

$$\frac{\partial E}{\partial x} = \frac{\partial F'}{\partial x} \frac{1}{b} \quad \text{and} \quad \frac{\partial F}{\partial y} = \frac{\partial E'}{\partial y} \frac{1}{f} - \frac{byf'}{f} \frac{\partial F'}{\partial y}.$$

and all other derivative terms, such as in the stresses, are converted to x, y derivatives by the chain rule.

Using operator slitting we can break the vector equation (35) into a sequence of single vector equations which can be used to define the solution. Define the operator L_x as defining the solution to the vector problem

$$\frac{\partial U}{\partial t} + \frac{\partial E}{\partial x} = 0.$$

Thus, L_x can be defined by the two step predictor-corrector formula

$$\begin{aligned} \text{predictor: } U_{i,j}^{**} &= U_{i,j}^* - \frac{\Delta t}{\Delta x} (E_{i+1,j}^* - E_{i,j}^*) \\ \text{corrector: } U_{i,j}^{**} &= \frac{1}{2} [U_{i,j}^* + U_{i,j}^{**} - \frac{\Delta t}{\Delta x} (E_{i,j}^{**} - E_{i-1,j}^{**})] \end{aligned}$$

where $U_{i,j}^{**} = L_x U_{i,j}^*$.

Similarly, we can define an operator L_y as the solution of the vector equation

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial y} = 0$$

where L_y is defined as

$$\begin{aligned} \text{predictor: } U_{i,j}^{**} &= U_{i,j}^* - \frac{\Delta t}{\Delta y} (F_{i+1,j}^* - F_{i,j}^*) \\ \text{corrector: } U_{i,j}^{**} &= \frac{1}{2} [U_{i,j}^* + U_{i,j}^{**} - \frac{\Delta t}{\Delta y} (F_{i,j}^{**} - F_{i-1,j}^{**})] \end{aligned}$$

where $U_{i,j}^{**} = L_y U_{i,j}^*$.

Finally, we define the operator L as the solution of the vector equation

$$\frac{\partial U}{\partial t} + H = 0$$

where L is defined by the modified Euler method or second order Runge-Kutta method

$$\begin{aligned} \text{predictor: } U_{i,j}^{**} &= -\Delta t H_{i,j}^* \\ \text{corrector: } U_{i,j}^{**} &= -U_{i,j}^* - \frac{\Delta t}{2} (H_{i,j}^* + H_{i,j}^{**}) \end{aligned}$$

where $U_{i,j}^{**} = L U_{i,j}^*$.

We can then define the following sequence of numerical calculations

$$U_{i,j}^{n+2} = L_x L_y L L_y L_x U_{i,j}^n. \quad (36)$$

That is we select a Δt which satisfies the CFL stability condition

$$(\Delta t)_{CFL} \leq \left(\frac{|V_x|}{\Delta x} + \frac{|V_y|}{\Delta y} + c \sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2}} \right)^{-1} \quad (37)$$

and $c = \sqrt{\frac{\gamma P}{\rho}}$ is the local speed of sound, and then perform the following sequence of calculations:

Step 1: Solve the system $U_{i,j}^1 = L_x U_{i,j}^n$.

Step 2: Solve the system $U_{i,j}^2 = L_y U_{i,j}^1$.

Step 3: Solve the system $U_{i,j}^3 = L U_{i,j}^2$.

Step 4: Solve the system $U_{i,j}^4 = L U_{i,j}^3$.

Step 5: Solve the system $U_{i,j}^5 = L_y U_{i,j}^4$.

Step 6: Solve the system $U_{i,j}^{n+2} = L_x U_{i,j}^5$.

Then redefine $U_{i,j}^n$, go to step 1 and repeat the calculations until the values $U_{i,j}^n$ stop changing. This then represents the steady state solution.

After calculating the vector

$$U_{i,j}^{(\text{steady state})} = (r\rho, r\rho V_r, r\rho V_z, r e_t)$$

we can calculate for all i, j values the quantities

$$\begin{aligned}\rho_{i,j} &= \frac{U(1)_{i,j}}{r_j} \\ V_{r i,j} &= \frac{U(2)_{i,j}}{r_j \rho_{i,j}} \\ V_{z i,j} &= \frac{U(3)_{i,j}}{r_j \rho_{i,j}}\end{aligned}$$

and since

$$U(4)_{i,j} = r_j e_{t i,j} = r_j \rho_{i,j} e_{i,j} + r_j \rho_{i,j} (V_{r i,j}^2 + V_{z i,j}^2)/2$$

we can determine the internal energy $e_{i,j}$ and hence the temperature $T_{i,j}$. In the model 2, two temperatures are determined since U will have dimension 5.

Initial and Boundary Conditions

We consider a one dimensional nozzle flow where the velocity V_z of the gas at any cross section is averaged over all cross sectional values. Let $A = A(z)$ denote the cross sectional area of the nozzle. We assume that the mass flow rate across any nozzle section is a constant and

$$Q_0 = \rho V_z A = \text{Constant},$$

so that we obtain using logarithmic derivatives that

$$\frac{d\rho}{\rho} + \frac{dV_z}{V_z} + \frac{dA}{A} = 0.$$

For isentropic gas flow we let H denote the enthalpy and use the Bernoulli theorem that

$$\frac{V_z^2}{2} + H = H_0 = \text{Constant},$$

together with the relations

$$pv^\gamma = \text{Constant}, \quad v = 1/\rho, \quad e_t = C_v T = \frac{pv}{\gamma - 1}, \quad H = e_t + pv = \frac{\gamma pv}{\gamma - 1}.$$

We can then write

$$\frac{d\rho}{\rho} = \frac{d\rho}{dp} \frac{dp}{\rho}$$

and use

$$\frac{dp}{d\rho} = \left(\frac{\partial p}{\partial \rho}\right)_s = c^2, \quad \frac{dp}{\rho} = dH = -V_z dV_z$$

to obtain

$$\frac{d\rho}{\rho} + \frac{dV_z}{V_z} = \frac{1}{c^2}(-V_z dV_z) + \frac{dV_z}{V_z} = \frac{dV_z}{V_z} \left(1 - \frac{V_z^2}{c^2}\right) = -\frac{dA}{A}.$$

Using

$$\frac{\rho}{p^{1/\gamma}} = \frac{\rho_0}{p_0^{1/\gamma}}$$

where ρ_0 and p_0 are the density and pressure while the gas is at rest, we write the enthalpy as

$$H = \frac{\gamma}{\gamma - 1} \frac{p}{\rho} = \frac{\gamma}{\gamma - 1} \left(\frac{p_0^{1/\gamma}}{\rho_0}\right) p^{(\gamma-1)/\gamma}.$$

Then the mass rate of flow $Q_0/A = \rho V_z$ becomes a function of pressure given by

$$\rho V_z = \rho [2(H_0 - H)]^{1/2} = \rho_0 \left(\frac{p}{p_0}\right)^{1/\gamma} \left(\frac{2\gamma}{(\gamma - 1)} \frac{p_0}{\rho_0} \left[1 - \left(\frac{p}{p_0}\right)^{1-1/\gamma}\right]\right)^{1/2}. \quad (15)$$

From this relation we can plot ρV_z vs p/p_0 . Note that $\rho V_z = 0$ when $p/p_0 = 1$ (gas at rest) and $p/p_0 = 0$ when gas expands into a vacuum. The maximum mass density occurs where $\frac{d\rho V_z}{dp} = 0$. This occurs at the throat where $V_z = c$. Since $A(z)$ is known, we can assume an initial value for Q_0 and then determine two pressures from equation (15) which can be plotted as a function of z . We adjust Q_0 until the two roots are equal at the throat. At this value of Q_0 we can then determine the exit (plenum) pressure p_p . If the exit pressure is any value greater than this critical value then shock waves can result and the flow could march backwards into the nozzle. We use the above analysis to determine starting entrance and exit pressures.

Our initial conditions are

At Entrance

The temperature, pressure (density), and initial velocities are specified according mass flow considerations. The radial velocity is selected in order that the radial velocity in the computational coordinates is initially zero. This requires that

$$V_{z_0} = \frac{V_{init} yf'(0)}{\sqrt{1 + (yf'(0))^2}} \quad V_{r_0} = \frac{V_{init}}{\sqrt{1 + (yf'(0))^2}}.$$

The temperature is initially set to a constant plenum temperature at all interior grid points. The plenum pressure is assumed constant at all interior grid points and the radial and axial velocities are set to zero.

Boundary Conditions

At the entrance (left boundary) the temperature, pressure and velocities are held constant. At the exit (right boundary) the pressure is held as the plenum pressure and the temperature and velocities are determined by extrapolation. Along the outside boundary of the nozzle the velocities are maintained as zero (no slip boundary condition) and the normal pressure and temperatures are maintained as zero. Along the centerline the radial velocity is zero while the temperature, axial velocity and density are determined by extrapolation.

APPENDIX A

List of Symbols

- \vec{b} = Body force vector per unit mass [*Newton/Kg*]
- C_{vrt} = Specific heat at constant volume for rotation-translation [*Joule/Kg K*]
- C_v = Specific heat at constant volume [*Joule/Kg K*]
- C_{vv} = Specific heat at constant volume for vibration [*Joule/Kg K*]
- $D_{i,j}$ = Rate of deformation tensor [s^{-1}]
- $\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{V} \cdot \nabla$ Material of substantial derivative
- e_t = Total energy [*Joule/m³ s*]
- e, e_r, e_v Internal energies [*Joule/m³ s*]
- h = Plank's constant [*J s*]
- h_1, h_2, h_3 Scale factors
- k = Boltzmann's constant [*J/K*]
- $m = \frac{W}{N_a}$ Molecular mass [*Kg*]
- N_a = Avogadro's number [mol^{-1}]
- \vec{q}_{rt} = Heat input due to rotation and translational energy [*Joule/m³ s*]
- \vec{q}_v = Heat input due to vibrational energy [*Joule/m³ s*]
- $\vec{q} = \vec{q}_{rt} + \vec{q}_v$ = Total heat energy [*Joule/m³ s*]
- P = Pressure [*Newton/m²*]
- R_0 = Universal gas constant [*Joule/K mole*]
- $R = R_0/W$ = Gas constant [*Joule/Kg K*]

List of Symbols

t	= time [s]
T, T_v	= Temperatures [K]
\vec{V}	= Velocity [m/s]
W	= Molecular weight of N_2 [Kg/mole]
η	= Viscosity coefficient [Kg/m s]
λ	= Second coefficient of viscosity [Kg/m s]
K_{rt}	= Thermal conductivity (rotation & translation) [W/m K]
K_v	= Thermal conductivity (vibration) [W/m s]
ρ	= Density [Kg/m ³]
τ	= Relaxation time [s]
τ_{ij}	= Stresses [Newton/m ²]
ϕ	= Characteristic vibration [K]
x, y	Computational coordinates
L_x, L_y, L	Operators

APPENDIX B

NOZZLE GEOMETRY

The nozzle geometry is illustrated in the Figure 1 where all dimensions are in millimeters.

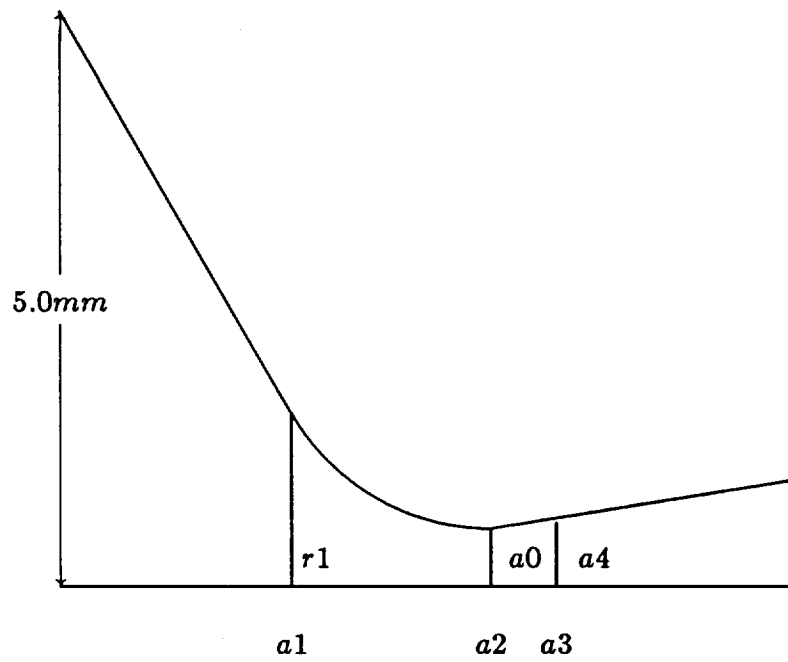


Figure 1. Nozzle Geometry

The throat radius is $a_0 = 0.5\text{mm}$, and the nozzle length is 350.0mm . The left end opening is 5.0mm . Starting at the point $(0, 5)$ on the left boundary, we move downward on a straight line having a slope of $-\sqrt{3}$. This line intersects a circle of radius 2.0mm centered at $(a_2, 2.5\text{mm})$ where the point a_2 is at the throat and is selected so that the slope of the line and the slope of the circle are the same at the point of intersection $z = a_1$. A point $a_3 > a_2$ is selected in order that a cubic spline can convert the circle into a straight line with slope of $\tan 8^\circ$. We write the equation of the circle as

$$(r - (a_0 + R))^2 + (z - a_2)^2 = R^2.$$

The equation of the line is

$$r - 5 = -(\tan 60^\circ)z.$$

At $z = a_2$ we require the slope of the circle to be zero, and at the point a_1 we require that the point (a_1, r_1) lie on the circle and further the slope of the circle equals the slope of the line. Solving the resulting equations we find that $a_1 - a_2 = -\sqrt{3}$,

$$a_1 = \frac{5 - (a_0 + R - \sqrt{R^2 - 3})}{\sqrt{3}} \quad \text{and} \quad a_2 = (8 - (a_0 + R - 1))/\sqrt{3}.$$

For $a_2 \leq z \leq a_3$ we must find the parameter a_3 such that a cubic spline converts the circle to a straight line. The cubic spline is represented

$$r = S_3(z) = A(z - a_2)^3 + B(z - a_2)^2 + C(z - a_2) + D \quad a_2 \leq z \leq a_3$$

and is subject to the end conditions that

$$S_3(a_2) = a_0, \quad S'_3(a_2) = 0, \quad S''_3(a_2) = 1/R, \quad S'_3(a_3) = \tan 8^\circ, \quad S''_3(a_3) = 0.$$

We find that

$$A = \frac{-1}{12R^2 \tan 8^\circ}, \quad B = \frac{1}{2R}, \quad C = 0, \quad D = a_0.$$

The equation of the nozzle is then given by

$$\begin{aligned} 0 \leq z \leq a_1, \quad r &= f(z) = -\sqrt{3}(z - a_2) + (a_0 + R - \sqrt{R^2 - 3} - 3) \\ a_1 \leq z \leq a_2, \quad r &= f(z) = a_0 + R - \sqrt{R^2 - (z - a_2)^2} \\ a_2 \leq z \leq a_3, \quad r &= f(z) = S_3(z) \\ a_3 \leq z \leq a_4, \quad r &= f(z) = a_4 + \tan 8^\circ(z - a_3) \end{aligned}$$

where

$$a_4 = S_3(a_3) \quad \text{and} \quad a_3 = a_2 + 2R \tan 8^\circ.$$